AI in the Sciences and Engineering HS 2025: Lecture 11

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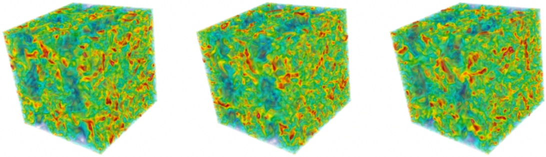
What we have learnt so far ?

- AIM: Learn PDEs using Deep Neural Networks
- Operator Learning: Learn the PDE Solution Operator from data.
- Examples: FNO, CNO, VIT, scOT etc.
- Very successful on PDEs on 2D Cartesian Domains !!
- Readily extended to time-dependent PDEs with all2all training.
- Extended to PDEs on Arbitrary domains with GNNs or GAOT.
- What are the remaining caveats ?

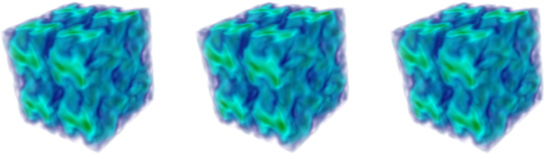
CAVEAT: What about PDEs with Chaotic Multiscale Solutions ?

3-D Navier-Stokes (Taylor-Green Vortex)

- Spectral Viscosity Method:



- Convolutional Fourier Neural Operator (C-FNO):



Why does this happen ?: Molinaro, SM et. al, 2025

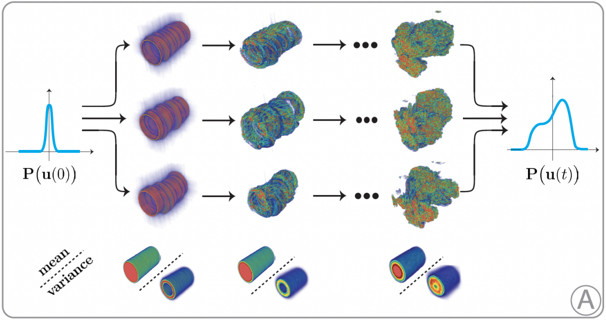
- Insensitivity of Neural Networks:

$$\Psi_\theta(u + \delta u) \approx \Psi_\theta(u), \; \delta u << 1$$

- DNNs are optimal at the Edge of Chaos: $\mathrm{Lip}(\Psi_\theta) \sim \mathcal{O}(1)$
- Spectral Bias of DNNs
- Bounded Gradients are essential for training with GD
- Implication $\Rightarrow$ DNNs will Collapse to Mean !!

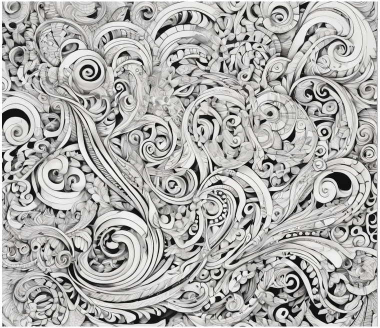
$$\mathbb{E}_{\delta\bar{u}} \|\Psi_\theta(\bar{u}^* + \delta\bar{u}) - \mathcal{S}(\bar{u}^* + \delta\bar{u})\|^2 \approx \mathbb{E}_{\delta\bar{u}} \|\Psi_\theta(\bar{u}^*) - \mathcal{S}(\bar{u}^* + \delta\bar{u})\|^2 \quad \text{(insensitivity hypothesis)}$$
$$= \|\Psi_\theta(\bar{u}^*) - \mathbb{E}_{\delta\bar{u}} \mathcal{S}(\bar{u}^* + \delta\bar{u})\|^2 + \mathrm{Var}_{\delta\bar{u}}[\mathcal{S}(\bar{u}^* + \delta\bar{u})]. \quad \text{(bias-variance decomposition)}$$

What can be done ?



- From Statistical Solutions: Fjordholm, Lanthaler, SM, 2016.
- Only Statistical Computation is feasible.
- Directly approximate the Conditional Distribution $P(u(t)|u_0)$

Generative AI to the Rescue ?

- Diffusion Models:
- Can generate Images and Videos with Small-scale details
- Need to provide Physical Correctness.
- Need to add Conditionalities

Conditional Sampling

Sample from $P(u \mid c)$ conditioned on input c.

Prompt

``A fox looking for his socks.''

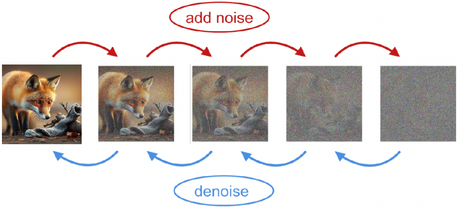
Input: conditioning c

Output: sample from $P(u \mid c)$

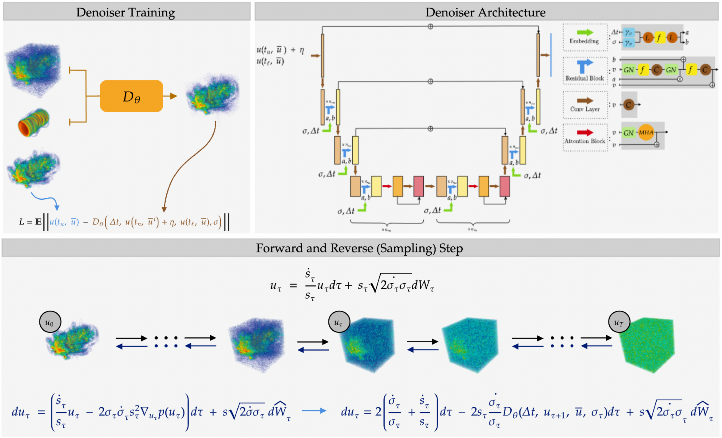
Noise Process and Denoising

- **Goal:** sample from $P(u \mid c)$
- **Noise process:** $u_\sigma = u + \sigma\eta$, $\eta \sim \mathcal{N}(0,1)$
- **Denoising:** revert the noise process

$$\mathcal{J}(D_\theta) := \mathbb{E}_{(u,c)}\mathbb{E}_{\eta,\sigma}\|D_\theta(u + \sigma\eta; c, \sigma) - u\|^2$$

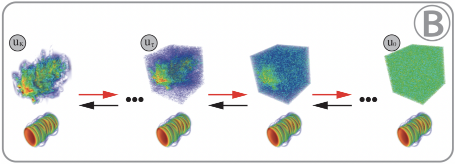


- Based on Conditional Score Based Diffusion Models



GenCFD algorithm of Molinaro et. al, SM, 2025

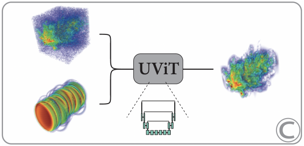
- Based on Conditional Score Based Diffusion Models



- Denoised with the Reverse SDE:

$$du_\tau = 2\left(\frac{\dot{\sigma}_\tau}{\sigma_\tau} + \frac{\dot{s}_\tau}{s_\tau}\right)d\tau - 2s_\tau\frac{\dot{\sigma}_\tau}{\sigma_\tau}D_\theta(\Delta t,\, u_{\tau+1},\, \overline{u},\, \sigma_\tau)d\tau + s\sqrt{2\dot{\sigma}_\tau\sigma_\tau}\, d\widehat{W}_\tau$$

- Denoiser minimizes $\mathbb{E}\|u(t_n, \bar{u}) - D_\theta(u(t_n, \bar{u}) + \eta, \bar{u}, \sigma)\|$



Why should this Work ?

- Recall Objective: Learn the Conditional Distribution:

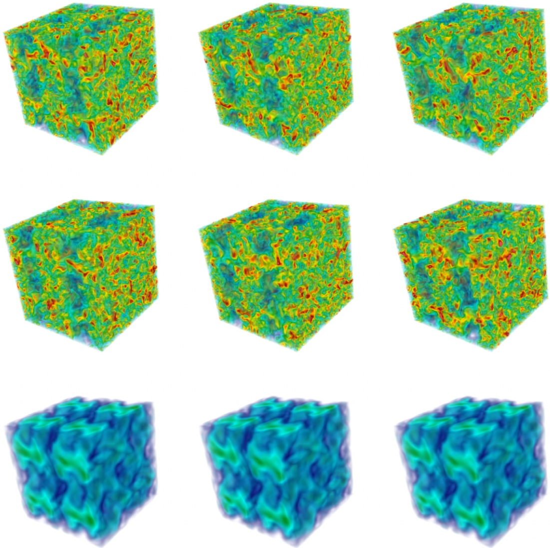
$$\text{Law}_{\delta\bar{u}}(\mathcal{S}(\bar{u}^* + \delta\bar{u}))$$

- A straightforward Calculation:

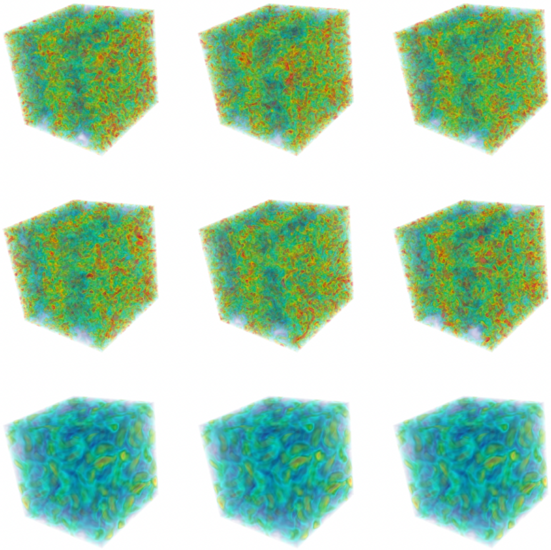
$$\begin{aligned}
\mathcal{J}(D_\theta) &= \mathbb{E}_{\delta\bar{u}}\mathbb{E}_\eta\left[\|D_\theta(\mathcal{S}(\bar{u}^* + \delta\bar{u}) + \eta; \bar{u}^* + \delta\bar{u}, \sigma) - \mathcal{S}(\bar{u}^* + \delta\bar{u})\|^2\right] \\
&\approx \mathbb{E}_{\delta\bar{u}}\mathbb{E}_\eta\left[\|D_\theta(\mathcal{S}(\bar{u}^* + \delta\bar{u}) + \eta; \bar{u}^*, \sigma) - \mathcal{S}(\bar{u}^* + \delta\bar{u})\|^2\right] \quad \text{(insensitivity hypothesis)} \\
&= \mathbb{E}_u\mathbb{E}_\eta\left[\|D_\theta(u + \eta; \bar{u}^*, \sigma) - u\|^2\right],
\end{aligned}$$

- is the Denoiser Training Objective to learn target distribution !!!
- Molinaro et. al, SM, 2025 formalize these arguments for Toy Models.

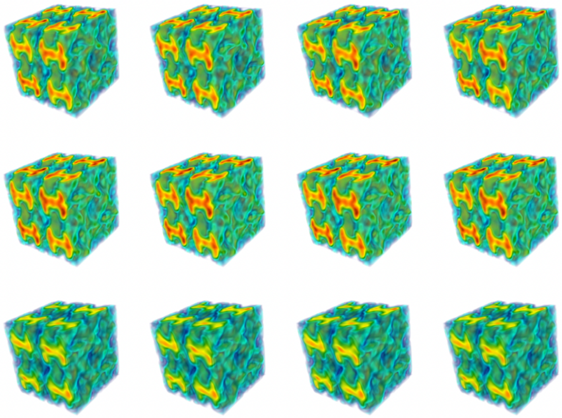
Taylor-Green: Kinetic Energy Samples



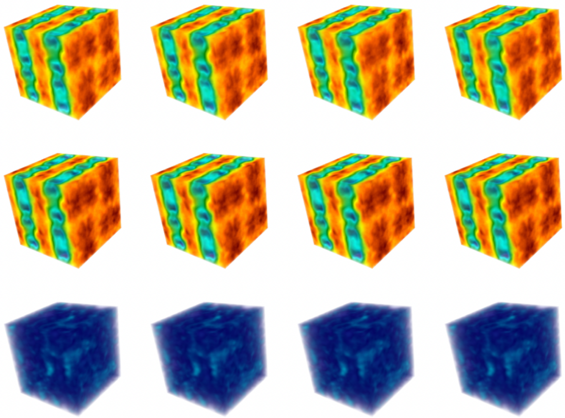
Taylor-Green: Vorticity Samples



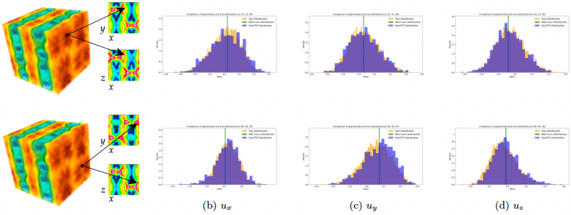
Taylor-Green: Mean



Taylor-Green: Variance

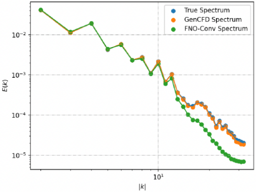


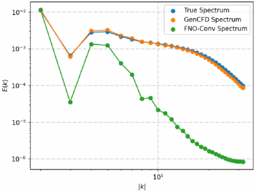
Taylor-Green: Point pdfs



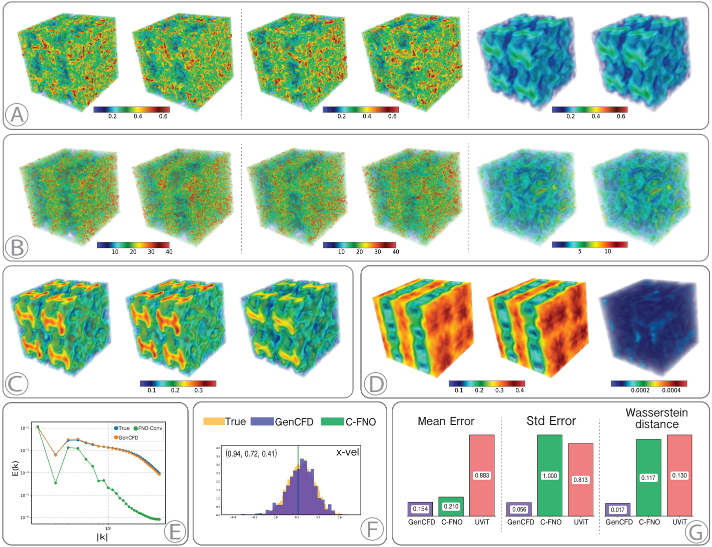
(a) Points (b) u_x (c) u_y (d) u_z

Taylor-Green: Spectra

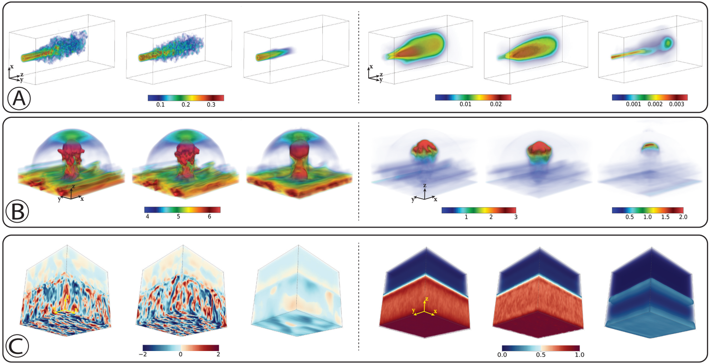




Taylor-Green Results with Micro-Macro setup

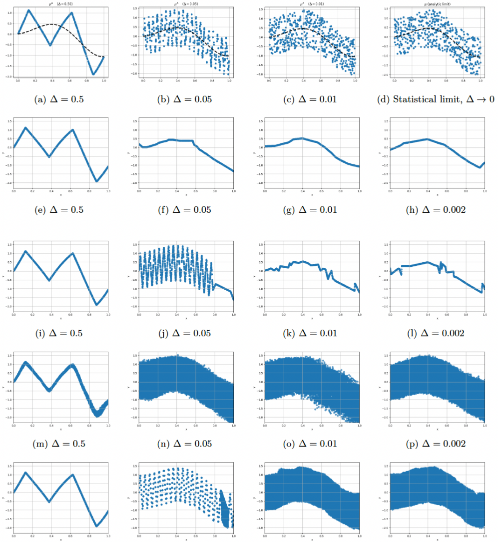


GenCFD works very well for Realworld Flows



- Nozzle Jet: 3.5 hrs (LBM) vs. GenCFD: 1.45s
- Cloud-Shock: 5 hrs (FVM) vs. GenCFD: 0.45s
- Conv. Boundary Layer: 13.3 hrs (FDM) vs. GenCFD: 3.8s

Results for a Toy Model



(a) $\Delta = 0.5$ (b) $\Delta = 0.05$ (c) $\Delta = 0.01$ (d) Statistical limit, $\Delta \to 0$

(e) $\Delta = 0.5$ (f) $\Delta = 0.05$ (g) $\Delta = 0.01$ (h) $\Delta = 0.002$

(i) $\Delta = 0.5$ (j) $\Delta = 0.05$ (k) $\Delta = 0.01$ (l) $\Delta = 0.002$

(m) $\Delta = 0.5$ (n) $\Delta = 0.05$ (o) $\Delta = 0.01$ (p) $\Delta = 0.002$

(q) $\Delta = 0.5$ (r) $\Delta = 0.05$ (s) $\Delta = 0.01$ (t) $\Delta = 0.002$

Perspective

- PDEs with Multi-scale Solutions.
- PDEs with sensitive dependence to Inputs.
- Fluid Flows
- Structural Mechanics (Fractures, Defects)
- Material Science
- Inverse Problems
- UQ
- Diffusion Models can work for all of them !!
- Other GenAI models: Rectified Flows, Normalizing Flows etc can be used too.